Phase 1 – Analytical and Numerical Solutions of Generalized Fokker-Planck Equations

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The overall objective of this NEER project at The University of New Mexico (in collaboration with a subcontractor at UCLA) was to develop improved analysis tools for the interaction and transport of highly collimated beams of charged particles in amorphous media. Such beams arise in several important applications which include medical (electron and ion radiotherapy), commercial (ion beam modification of materials), environmental (accelerator transmutation of waste) and defense (accelerator production of tritium). A robust predictive/analytical capability would then be greatly beneficial and provide a cost effective alternative to expensive experiments and cumbersome Monte Carlo simulations..

The specific goals are to develop theoretical and deterministic numerical approaches for analyzing the spatial, angular and energy spreading of a pencil beam (monoenergetic, monodirectional and spatially localized) of charged particles as it penetrates the target material. While the linear Boltzmann or transport equation provides a valid and accurate formulation of this problem, the highly forward peaked scattering characteristic of charged particle interactions renders this approach intractable for analytical work and impractical for direct numerical solution. On the other hand, the accuracy of the popular Fokker-Planck and Fermi approximations to the transport equation has been shown to be restricted to the vicinity of the beam axis with the accuracy rapidly degrading with increasing transverse or radial distance. This is a consequence of two inherent approximations in these models: the neglect of large angle scattering and the assumption of near collimation of the beam as it traverses the medium.

To improve these models, we have proposed and investigated a Generalized Fokker-Planck formalism to accommodate the effects of larger angle scattering, as well as a novel approach to relaxing the near collimation assumption. During the course of these investigations other interesting and relevant problems arose which required novel solution approaches to be developed. The accomplishments of this phase of the project are described below.

1. The Generalized Fokker-Planck model in broad beam geometry. .

We propose the Generalized Fokker-Planck (GFP) model for pencil beam transport under conditions when the scattering is not sufficiently forward peaked for the classic Fokker-Planck (FP) approximation to the scattering integral to be valid. That is, while $1-\overline{m} << 1$ may hold, the rate of the cross section fall-of with scattering angle may not be sufficiently rapid for the FP representation to be accurate. It is then reasonable to consider higher order FP expansions of the scattering integral to account for larger scattering angles. Truncating this expansion yields the GFP equation which for broad beam incidence may be expressed as

$$\mu \frac{\partial \psi}{\partial z} = \sum_{k=1}^{K} \alpha_k L^k \psi \ ,$$

where L is the Fokker -Planck scattering operator and the higher order FP expansion has been truncated after K terms. The coefficients appearing in the sum above depend on the various angular moments of the differential cross section and the presumption is that for a sufficiently forward peaked scattering cross section the sum will converge rapidly and provide a means of assessing the effects of larger angle scattering on the scalar flux, which is the physical quantity of interest. We solve the GFP equation in a slab that is thin when measured in transport mean free paths (but nevertheless optically very thick in scattering mean free paths) by considering the $(1-\mu)^n$ – moments of the angular flux in conjunction with a closure relationship. We have earlier demonstrated the effectiveness of the method in relation to the FP model, which is a special case of the GFP equation with K=1, in particular showing its superiority over the Legendre expansion for this class of problems. Implementation of the solution algorithm required high numerical precision for which MAPLE proved extremely effective. Numerical results for the scalar flux were obtained using this method for the FP, GFP and exact transport models. For highly forward peaked scattering, $(1-\overline{\mu}) = 10^{-3}$, the FP approximation is reasonably accurate but the accuracy rapidly erodes with increasing $(1-\overline{\mu})$. The GFP model, on the other hand, gives consistently accurate results when enough terms in the higher order FP expansion are retained. This expansion is in fact an asymptotic expansion and must be truncated at a turning point which depends on $(1-\overline{\mu})$.Further investigation of higher order terms in the GFP expansion will be considered in Phase 2 of this project.

2. Modification of the classic Fermi-Eyges formalism for the pencil beam problem to achieve greater accuracy for large radii.

The Fermi-Eyges formula, while simple, elegant and explicit, turns out to be very inaccurate for large radii (radial locations comparable to axial depth), i.e., for large beam deflections. This is, of course, not unexpected since the near-collimation assumption is inconsistent with large beam deflections. In this task we successfully developed a large deflection modification of the Fermi-Eyges formula which retains the simplicity of the classic Fermi-Eyges formula but yields dramatic improvements in accuracy. The basis of this idea is to relax the near-collimation assumption, which is a straight ahead approximation (i.e., $\mu = 1$) by introducing μ^* a characteristic value of μ which depends on the spatial coordinates r and z. We now introduce the Fermi approximation to the scattering which, in the straight ahead approximation, nominally replaces scattering on the unit sphere with angular diffusion in the plane tangent to this sphere at $\mu = 1$. Now, however, we have to proceed more generally and approximate the spherical Laplacian by the Laplacian in the plane tangent to the sphere at μ^* and φ^* (the characteristic azimuthal angle). This was successfully derived and a useful form for evaluation, subject only to the specification of μ^*, was obtained by averaging over the characteristic azimuthal angle.

To specify the functional form of μ^* we argue as follows. For a particle to find itself at a large radial coordinate one or more large angle scattering collisions must have occurred. Since large angle scatterings are rare, the most likely scenario is that a single large angle scattering will occur, followed by many highly forward peaked collisions. Further, this large angle collision most likely occurs just as the particle enters the slab, for then the scattering angle needed to achieve the a given r/z is the smallest, in contrast to a scattering event taking place deeper in the slab. Based on these arguments, we equate the characteristic phase space angle $q^* = \cos^{-1}(m^*)$ to the geometric angle $\Theta^* = \tan^{-1}(r/z)$ and use this to evaluate the modified Fermi-Eyges formula.

Numerical results show that the modified Fermi-Eyges formula, when compared against exact Monte Carlo simulations and the original Fermi-Eyges theory, gives dramatically improved results for large radial distances. For instance, the error at r=1.2 mean free paths is reduced from more than 6 orders of magnitude to less than a factor of 2. An important factor in achieving this enhanced accuracy is that the modified Fermi-Eyges formula shows algebraic fall-off at large radii compared to the Gaussian Fermi-Eyges result. While the improvements realized were the result of an ad hoc correction introduced in the classic Fermi-Eyges theory, the large radius errors were dramatically curtailed. In the second phase of this investigation a more rigorous approach to developing a modified Fermi-Eyges theory will be considered.

3. A quadratic discontinuous Galerkin finite element code with Fokker-Planck scattering and continuous slowing down energy loss.

Closed form analytic solutions to the transport equation and its variants provide valuable insight into the spreading and energy loss of an incident charged particle beam as it penetrates the medium and, under certain circumstances, may even be used directly in applications, e.g., the Fermi-Eyges solution is used in radiation therapy treatment planning algorithms. However, as these solutions do not represent exact solutions of the underlying equations, but rather are solutions to approximate equations, the errors can only be quantified when compared against benchmark solutions. Benchmarks are typically generated using Monte Carlo simulations but these tend to be slow and cumbersome. With increasing computational sophistication, in both hardware and software, deterministic numerical solution approaches are becoming viable. With the goal of eventually developing a 3D deterministic code for pencil beam problems, we have begun investigations into high order accurate finite element solutions of the 1D or broad beam geometry problem with Fokker-Planck scattering and continuous slowing down energy loss.

In Phase 1 of this project, we initially developed and implemented the linear and bilinear discontinuous finite element schemes, in space and energy, as well as the nonlinear exponential discontinuous and linear characteristic methods. The FP angular operator was discretized using standard Gauss quadrature as well as a logarithmic angular quadrature dense around the incident particle direction. Solutions for the energy spectrum as well as the dose profile were obtained and compared. While the nonlinear scheme was the most robust, in that it yields unconditionally positive solutions for the problems considered, it displayed the most numerical straggling and gave the poorest resolution of the Bragg peak and the sharply varying energy spectra. The bilinear discontinuous and characteristic methods gave better resolution and although the schemes do not yield unconditionally positive solutions, any negativities are rapidly damped. The linear discontinuous scheme was better than the exponential but not as good as the other linear schemes. However, all schemes gave acceptable accuracy only on extremely refined grids for this class of problems with highly forward peaked scattering and dominant CSD energy loss. We next implemented a higher order accurate quadratic discontinous scheme in space and energy, which gave dramatically improved resolution of the energy spectra and dose distribution. This is in part due to the greater degree of curvature provided by a quadratic polynomial trial function. Accuracy was achieved on coarser grids than the other methods investigated. We conclude that a quadratic representation of the flux at a minimum must be used for these problems which are characterized by small angular scattering and strong CSD energy losses. To establish the true efficacy of this method a generalized polynomial finite element setting should be explored and this will be considered in Phase 2.

4. A multigroup downscatter-only model for charged particle energy loss straggling.

In the course of our investigations into the transport of high energy pencil beams of charged particles it became clear that, especially for energetic ions, the continuous slowing down (CSD) model of energy loss is inadequate and that the effect of energy loss fluctuations, known as electronic energy loss straggling, must be accounted for in order to accurately describe the energy spectrum of the beam as it traverses the medium. However, the small energy loss per collision between an incident ion and a target electron cannot be effectively resolved using standard multigroup methods. While a Fokker-Planck model of energy loss straggling which gives the correct mean-squared energy loss can be developed, it possesses unphysical features like upscatter and, furthermore, it is an inappropriate model for incorporating in a transport code based on a standard space–energy sweep algorithm.

We have developed a multigroup model of energy loss straggling arising from inelastic energy loss fluctuations in the incident ion energy. Straggling is incorporated through an adjacent-group down-scatter only cross section, defined such that the mean square energy loss is preserved. The absence of upscatter in our novel approach makes it superior to existing approaches which treat straggling as a diffusive process in energy and have to deal with unphysical upscattering. In the context of the space-energy sweep algorithm in transport codes, outer iterations become necessary to treat these upscatter collisions. This complication is avoided in our approach which treats straggling as strictly a down-scatter process while ensuring that both the mean and mean squared energy loss is preserved. The resulting effective transport equation is computationally more efficient to solve than one based on the exact but nearly singular differential cross section. The electronic straggling coefficients, describing the mean square energy loss, for arbitrary incident ion-target atom combinations are taken from recent state-of-the-art semi-empirical compilations, which incorporate charge exchange and correlation corrections to the well known Bohr result. This model, as well as it's generalization to preserve higher energy loss moments, will be implemented in our arbitrary order finite element code with angular scattering which will be developed during Phase 2 of this project.

5. A renormalized Generalized Fokker-Planck theory of energy loss straggling.

Our multigroup model of energy loss straggling, while computationally efficient and accurate, preserves only the mean and mean-squared energy loss and not higher moments of energy loss. For thin target applications, such as proton radiography, this provides an adequate resolution of the energy spectrum of the transmitted beam but the preservation of higher moments becomes necessary when significant beam attenuation occurs. As mentioned in the previous section, additional multigroup cross sections may be defined but this procedure is not entirely rigorous, although the approach is effective. We have developed a novel and more rigorous approach to constructing simpler energy loss kernels which can preserve a prescribed number moments. Our approach begins with first developing a higher order Fokker-Planck expansion of the energy loss collision integral in the transport equation. If all terms in this expansion are retained then this representation will preserve all energy transfer moments. In practice the series must be truncated at some finite order and so the resulting Generalized Fokker-Planck representation will preserve a finite number of these moments. However, we have shown that the GFP model is unstable for any truncation order beyond the second, i.e., beyond strictly Fokker-Planck. The essence of our idea is that the requisite number of terms in this expansion are retained, depending on the desired number of energy loss moments to be preserved, and the rest are approximated to yield a stable expansion. However, this procedure must be carried out in such a way that the renormalized expansion is easier to deal with. A systematic approach to this is to seek a Pade or rational function representation of the GFP operator expansion such that the series expansion of the former matches the GFP expansion up to the truncated order. We have shown for low order truncations, with energy independent physical parameters, that the renormalized GFP expansion is equivalent to an effective collision integral which is considerably smoother than the original integral and hence is computationally more efficient. Furthermore, closed form solutions agree extremely well with the multigroup model and exact Monte Carlo simulations. In Phase 2 of this project, we propose to generalize this renormalization procedure to retain higher energy loss moments and to develop a practical algorithm for numerical solution with realistic data.